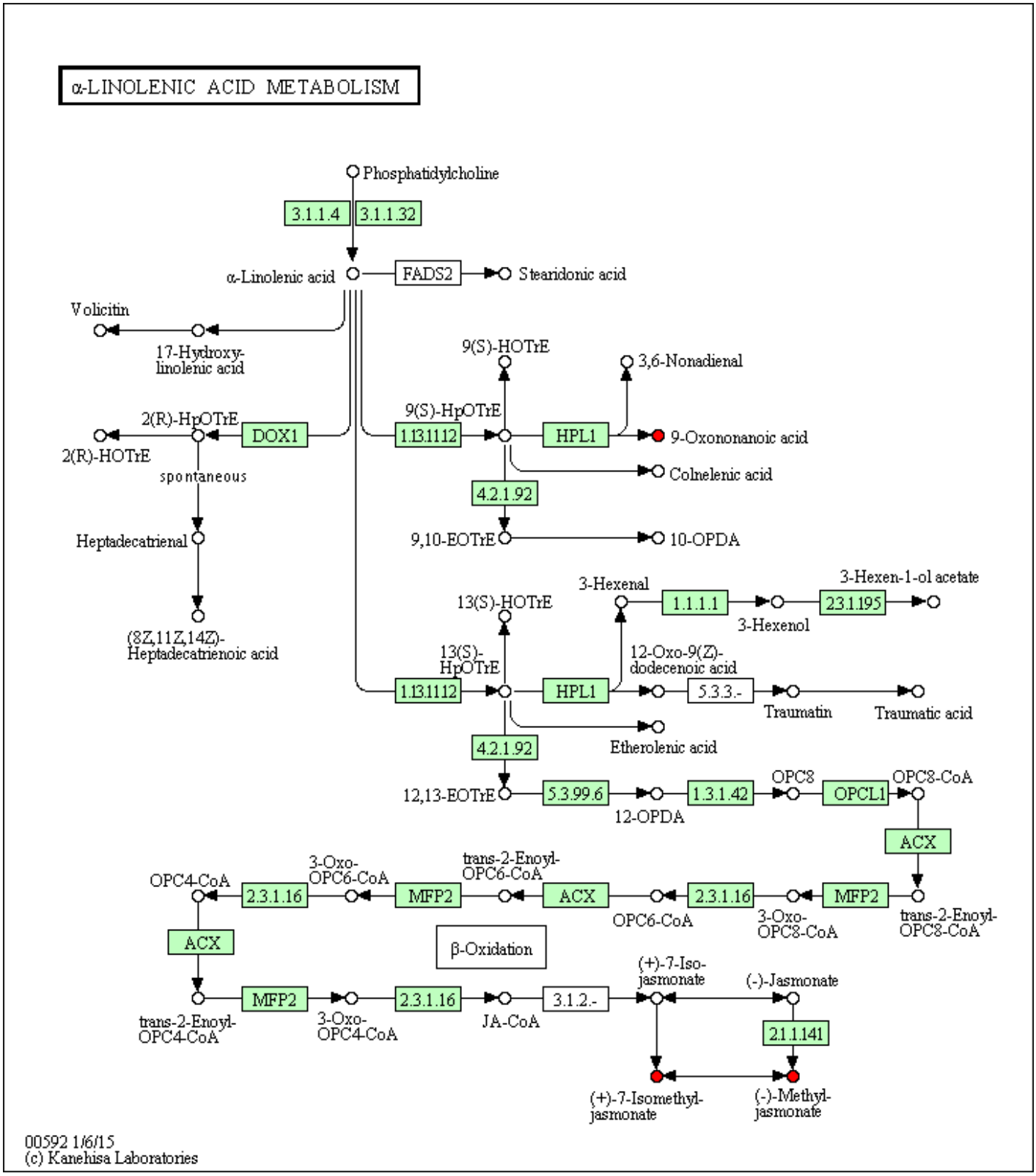
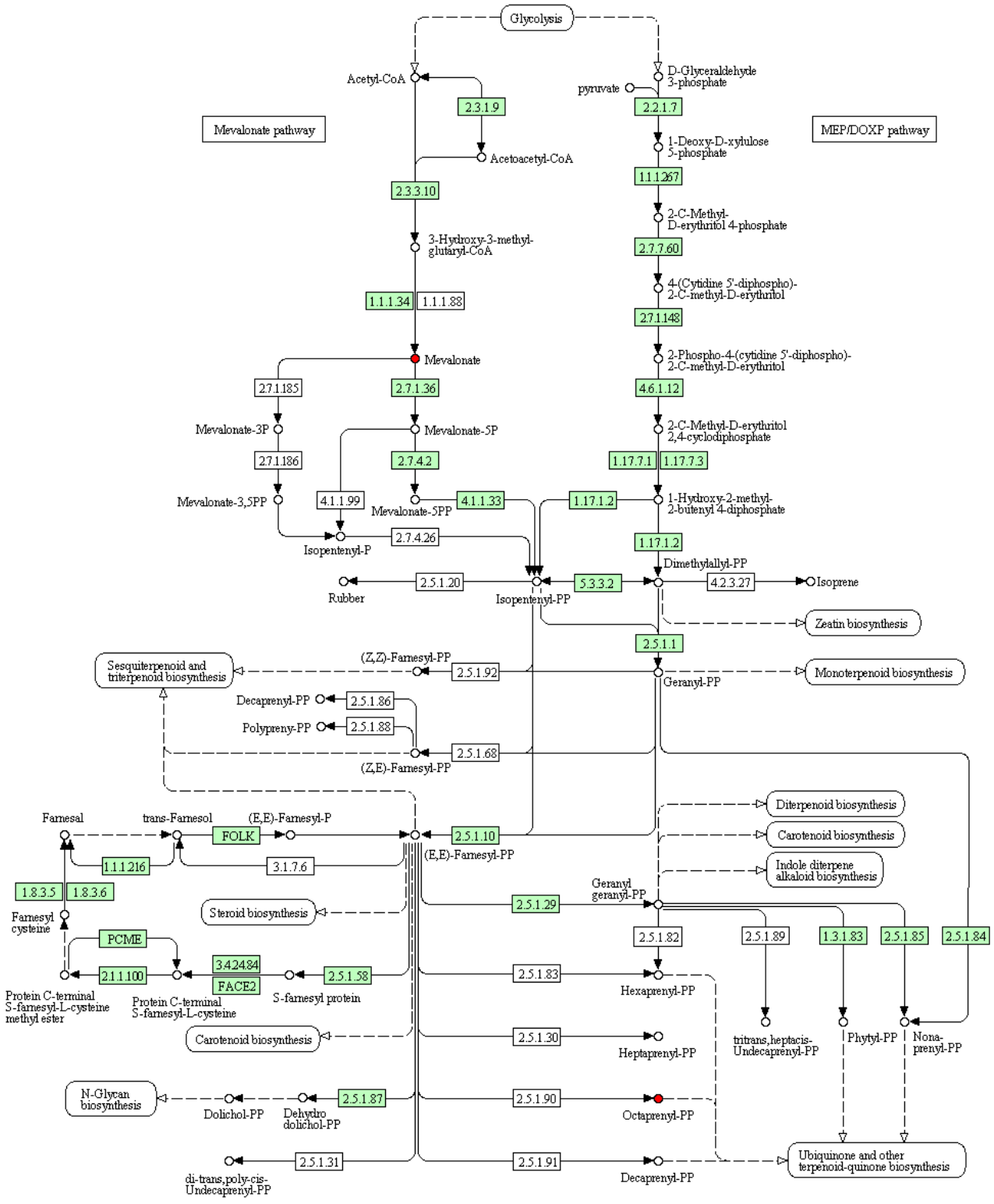
Supplementary figure 2: Compounds putatively identified in pathways in positive ionization. Red dots represent compounds identified by exact mass in the linolenic acid metabolism, terpenoid backbone biosynthesis, monoterpenoid biosynthesis, diterpenoid biosynthesis, limonene and pinene degradation, pentose phosphate and carbon metabolism pathways.



TERPENOID BACKBONE BIOSYNTHESIS



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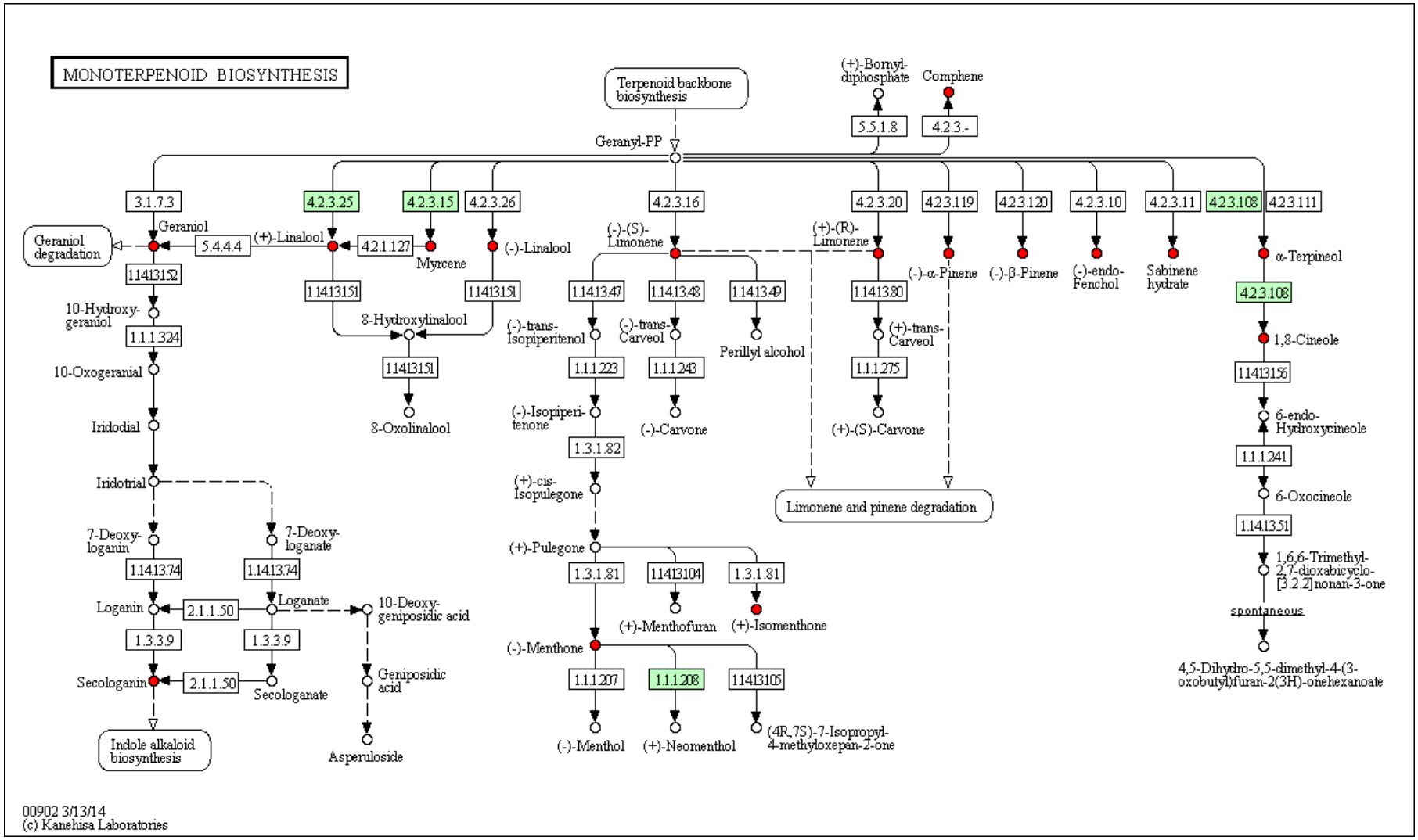
MONOTERPENOID BIOSYNTHESIS
Terpenoid backbone biosynthesis
Geranyl-PP
(+)-Bornyl-diphosphate
Comphene
5.5.1.8
4.2.3.-
3.1.7.3
4.2.3.25
4.2.3.15
4.2.3.26
4.2.3.16
4.2.3.20
4.2.3.119
4.2.3.120
4.2.3.10
4.2.3.11
4.2.3.108
4.2.3.111
Geraniol
Geraniol degradation
5.4.4.4
(+)-Linalool
4.2.1.127
Myrcene
(-)-Linalool
(-)-(S)-Limonene
(+)-(R)-Limonene
(-)-α-Pinene
(-)-β-Pinene
(-)-endo-Fenchol
Sabinene hydrate
α-Terpineol
1.14.13.152
1.14.13.151
1.14.13.151
1.14.13.47
1.14.13.48
1.14.13.49
1.14.13.80
4.2.3.108
10-Hydroxy-geraniol
8-Hydroxylinalool
(-)-trans-Isopiperitenol
(-)-trans-Carveol
Perillyl alcohol
(+)-trans-Carveol
1,8-Cineole
1.1.1.324
1.14.13.151
1.1.1.223
1.1.1.243
1.1.1.275
1.14.13.156
10-Oxogeranial
8-Oxolinalool
(-)-Isopiperi-tenone
(-)-Carvone
(+)-(S)-Carvone
6-endo-Hydroxycineole
Iridodial
1.3.1.82
1.1.1.241
Iridotrial
(+)-cis-Isopulegone
Limonene and pinene degradation
6-Oxocineole
7-Deoxy-loganin
7-Deoxy-loganate
(+)-Pulegone
1.14.13.74
1.14.13.74
1.3.1.81
1.14.13.104
1.3.1.81
1.14.13.51
Loganin
2.1.1.50
Loganate
10-Deoxy-geniposidic acid
(+)-Menthofuran
(+)-Isomenthone
1,6,6-Trimethyl-2,7-dioxabicyclo-[3.2.2]nonan-3-one
1.3.3.9
1.3.3.9
(-)-Menthone
spontaneous
Secologanin
2.1.1.50
Secologanate
Geniposidic acid
1.1.1.207
1.1.1.208
1.14.13.105
4,5-Dihydro-5,5-dimethyl-4-(3-oxobutyl)furan-2(3H)-onehexanoate
Indole alkaloid biosynthesis
Asperuloside
(-)-Menthol
(+)-Neomenthol
(4R,7S)-7-Isopropyl-4-methyloxepan-2-one
00902 3/13/14
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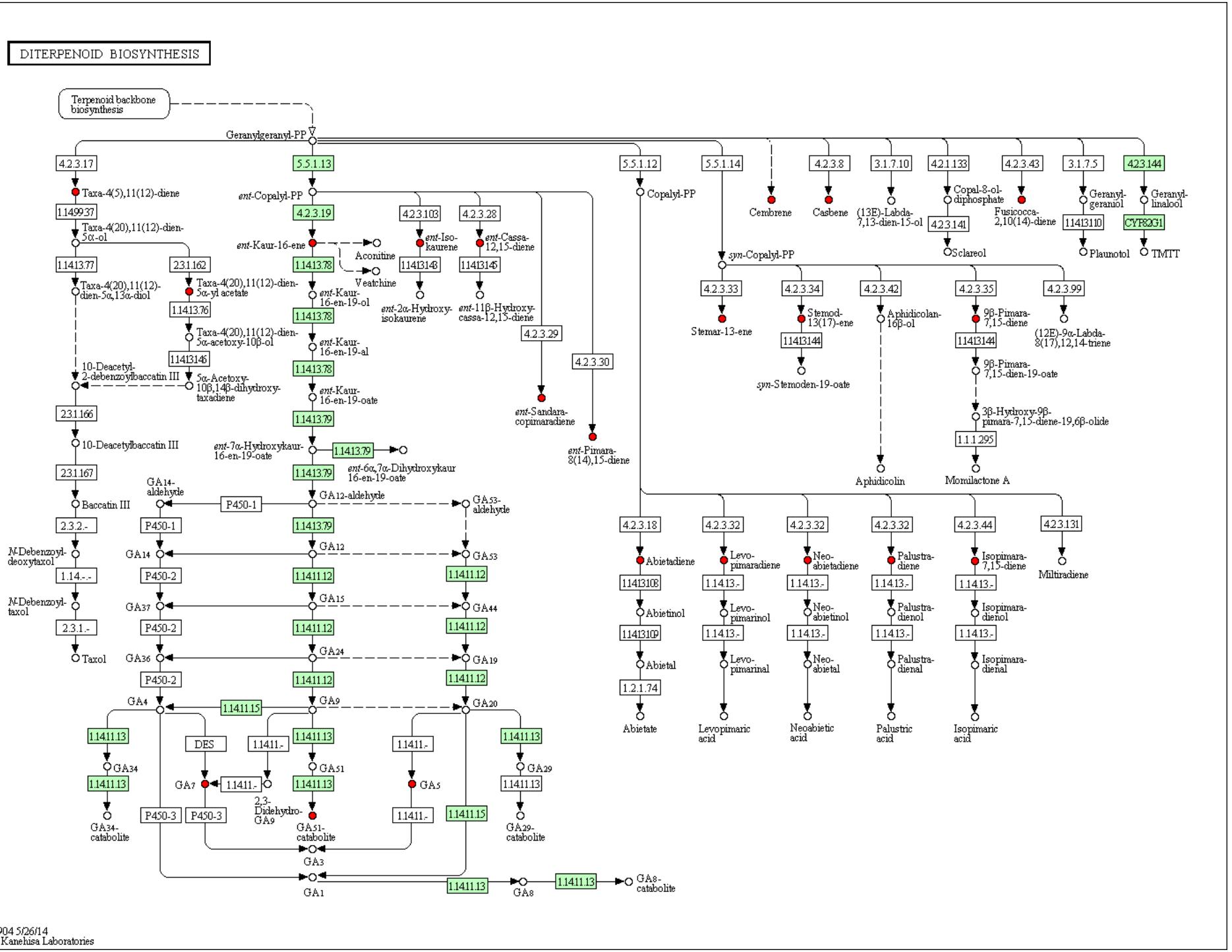

00904 5/26/14
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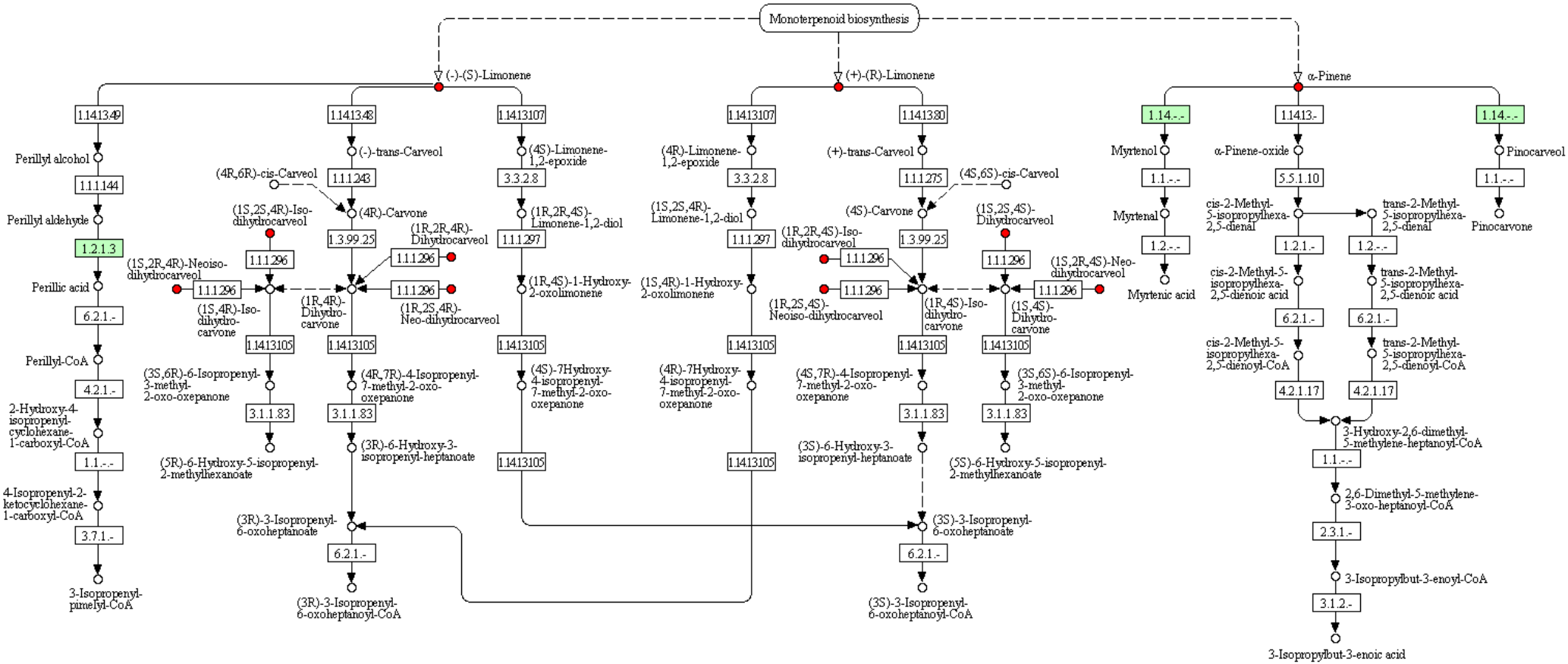
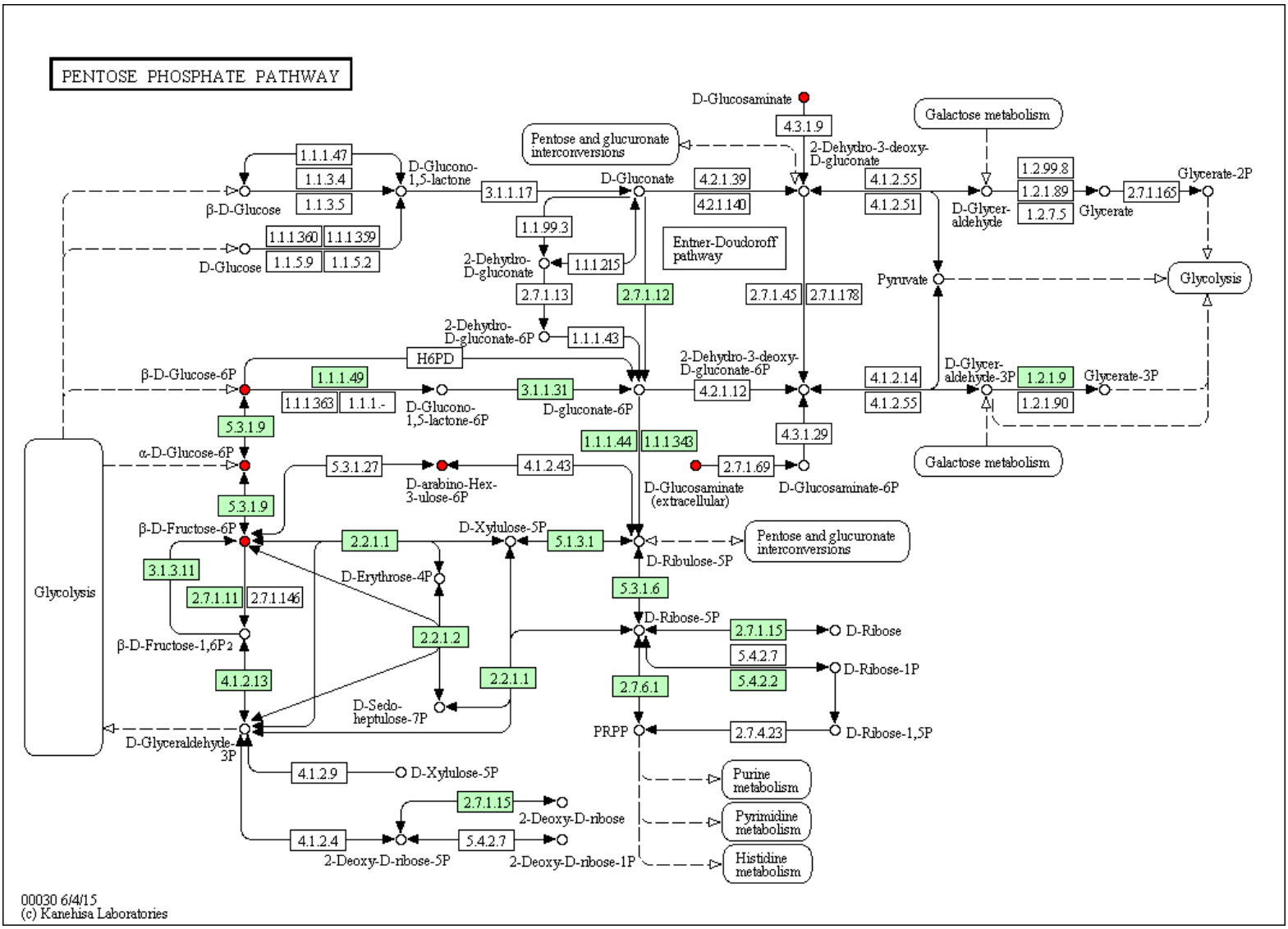
LIMONENE AND PINENE DEGRADATION



00903 5/19/15


PENTOSE PHOSPHATE PATHWAY
D-Glucosaminate
4.3.1.9
Galactose metabolism
Pentose and glucuronate interconversions
2-Dehydro-3-deoxy-D-gluconate
1.1.1.47
1.1.3.4
1.1.3.5
D-Glucono-1,5-lactone
3.1.1.17
D-Gluconate
4.2.1.39
4.2.1.140
4.1.2.55
4.1.2.51
1.2.99.8
1.2.1.89
1.2.7.5
Glycerate-2P
2.7.1.165
Glycerate
D-Glycer-aldehyde
β-D-Glucose
1.1.1.360
1.1.1.359
1.1.5.9
1.1.5.2
D-Glucose
1.1.99.3
2-Dehydro-D-gluconate
1.1.1.215
Entner-Doudoroff pathway
2.7.1.13
2.7.1.12
2.7.1.45
2.7.1.178
Pyruvate
Glycolysis
2-Dehydro-D-gluconate-6P
1.1.1.43
H6PD
2-Dehydro-3-deoxy-D-gluconate-6P
β-D-Glucose-6P
1.1.1.49
1.1.1.363
1.1.1.-
D-Glucono-1,5-lactone-6P
3.1.1.31
D-gluconate-6P
4.2.1.12
4.1.2.14
4.1.2.55
D-Glycer-aldehyde-3P
1.2.1.9
1.2.1.90
Glycerate-3P
5.3.1.9
1.1.1.44
1.1.1.343
4.3.1.29
α-D-Glucose-6P
5.3.1.27
4.1.2.43
2.7.1.69
D-arabino-Hex-3-ulose-6P
D-Glucosaminate (extracellular)
D-Glucosaminate-6P
Galactose metabolism
5.3.1.9
β-D-Fructose-6P
2.2.1.1
D-Xylulose-5P
5.1.3.1
Pentose and glucuronate interconversions
D-Ribulose-5P
3.1.3.11
D-Erythrose-4P
Glycolysis
2.7.1.11
2.7.1.146
5.3.1.6
D-Ribose-5P
2.7.1.15
D-Ribose
β-D-Fructose-1,6P2
2.2.1.2
5.4.2.7
D-Ribose-1P
4.1.2.13
2.2.1.1
5.4.2.2
2.7.6.1
D-Sedo-heptulose-7P
PRPP
2.7.4.23
D-Ribose-1,5P
D-Glyceraldehyde-3P
4.1.2.9
D-Xylulose-5P
Purine metabolism
2.7.1.15
2-Deoxy-D-ribose
Pyrimidine metabolism
4.1.2.4
5.4.2.7
2-Deoxy-D-ribose-5P
2-Deoxy-D-ribose-1P
Histidine metabolism
00030 6/4/15
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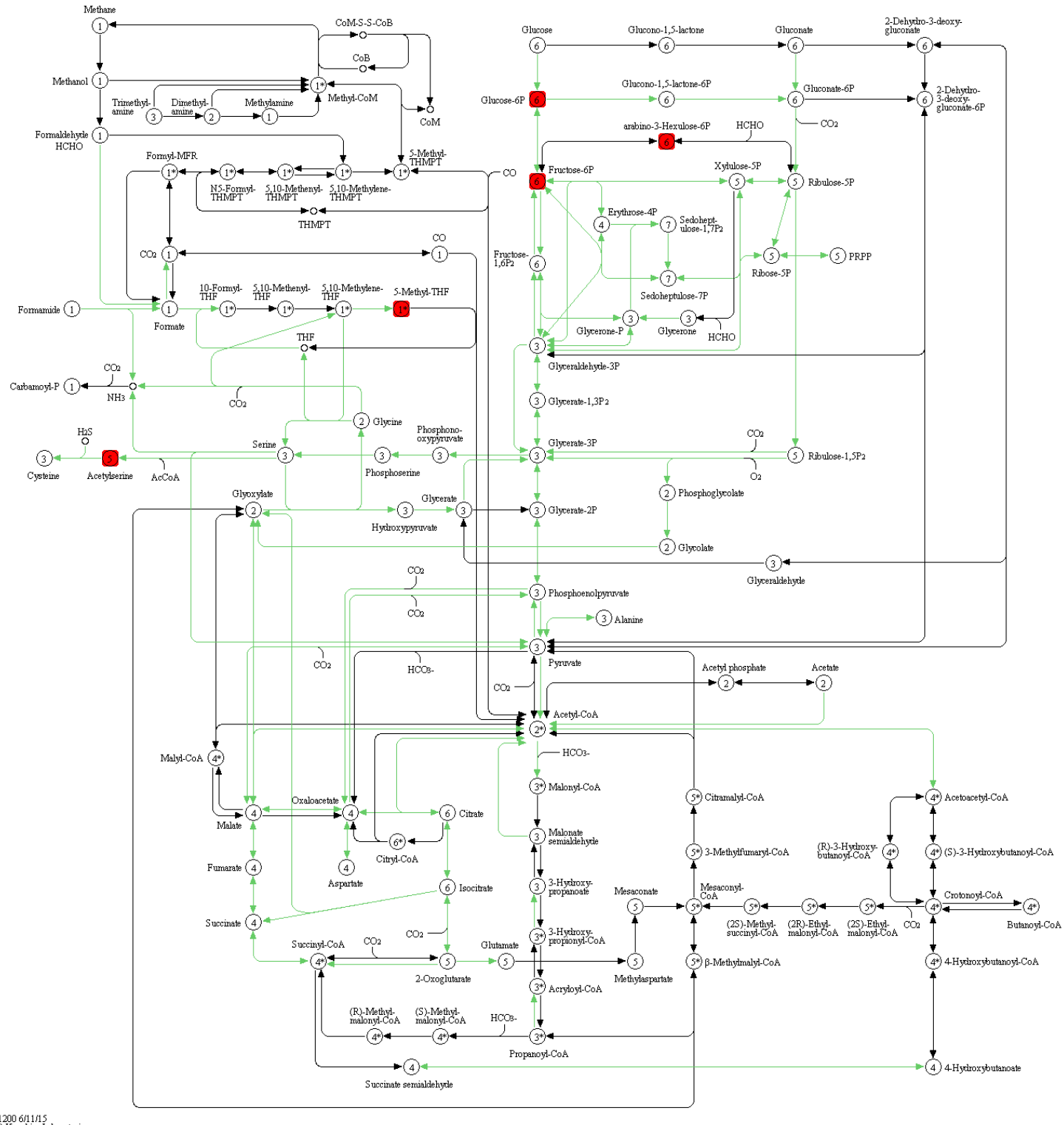
CARBON METABOLISM
Methane
CoM-S-S-CoB
CoB
Methanol
Trimethyl-amine
Dimethyl-amine
Methylamine
Methyl-CoM
CoM
Formaldehyde HCHO
Formyl-MFR
5-Methyl-THMPT
N5-Formyl-THMPT
5,10-Methenyl-THMPT
5,10-Methylene-THMPT
THMPT
CO
CO2
Formamide
Formate
10-Formyl-THF
5,10-Methenyl-THF
5,10-Methylene-THF
5-Methyl-THF
THF
Carbamoyl-P
NH3
H2S
Cysteine
Acetylserine
AcCoA
Serine
Glycine
Phosphono-oxypyruvate
Phosphoserine
Glyoxylate
Glycerate
Hydroxypyruvate
Glycerate-3P
Glycerate-2P
Glycerate-1,3P2
Phosphoglycolate
Glycolate
Glyceraldehyde
Phosphoenolpyruvate
Alanine
Pyruvate
HCO3-
Acetyl phosphate
Acetate
Acetyl-CoA
Malyl-CoA
Oxaloacetate
Malate
Citrate
Citryl-CoA
Fumarate
Aspartate
Isocitrate
Succinate
Succinyl-CoA
2-Oxoglutarate
Glutamate
Malonyl-CoA
Malonate semialdehyde
3-Hydroxy-propanoate
3-Hydroxy-propanoyl-CoA
Acryloyl-CoA
Propanoyl-CoA
Methylaspartate
Mesaconate
Mesaconyl-CoA
(2S)-Methyl-succinyl-CoA
(2R)-Ethyl-malonyl-CoA
(2S)-Ethyl-malonyl-CoA
Citramalyl-CoA
3-Methylfumaryl-CoA
β-Methylmalyl-CoA
(R)-Methyl-malonyl-CoA
(S)-Methyl-malonyl-CoA
Succinate semialdehyde
(R)-3-Hydroxy-butanoyl-CoA
Acetoacetyl-CoA
(S)-3-Hydroxybutanoyl-CoA
Crotonoyl-CoA
Butanoyl-CoA
4-Hydroxybutanoyl-CoA
4-Hydroxybutanoate
Glucose
Glucono-1,5-lactone
Gluconate
2-Dehydro-3-deoxy-gluconate
Glucose-6P
Glucono-1,5-lactone-6P
Gluconate-6P
2-Dehydro-3-deoxy-gluconate-6P
arabino-3-Hexulose-6P
HCHO
Fructose-6P
Xylulose-5P
Ribulose-5P
Erythrose-4P
Sedohept-ulose-1,7P2
Fructose-1,6P2
Ribose-5P
PRPP
Sedoheptulose-7P
Glycerone-P
Glycerone
Glyceraldehyde-3P
Ribulose-1,5P2
O2
01200 6/11/15
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